Analytical expressions for the local-field factor $G(q)$ and the exchange-correlation kernel $K_{xc}(r)$ of the homogeneous electron gas.

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We present an analytical expression for the local field factor $G(q)$ of the homogeneous electron gas which reproduces recently published Quantum Monte–Carlo data by S. Moroni, D.M. Ceperley, and G. Senatore [Phys. Rev. Lett. **75**, 689 (1995)], reflects the theoretically known asymptotic behaviours for both small and large q limits, and allows to express the exchange-correlation kernel K_{xc} analytically in both the direct and reciprocal spaces. The last property is particularly useful in numerical applications to real solids.

31.15.Ew, 05.30.Fk

The static local field factor $G(q)$ of the homogeneous electron gas (HEG) is an important quantity because it represents the extent to which the particle interactions affect the exchange and correlation properties of this idealized system. The importance of $G(q)$ in calculating the properties of real materials stems from the fact that it can be used as a key input in density functional calculations [1,2]. In fact, approximations of the unknown exchange-correlation energy functional of real (inhomogeneous) systems involve the second functional derivative of $E_{xc}[n]$, or exchange correlation kernel

$$K_{xc}(n_o;|\mathbf{r}-\mathbf{r}^{'}|)=\frac{\delta^2 E_{xc}[n]}{\delta n(\mathbf{r})\delta n(\mathbf{r}^{'})}|_{n_o}, \tag{1}$$

where n_o is the HEG density. On the other hand, the local field factor and the exchange correlation kernel are simply related in Fourier space by [3]:

$$\begin{aligned} K_{xc}^{FT}(q) &\equiv \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} K_{xc}(r) \\ &= -v_c(q)G(q), \end{aligned} \tag{2}$$

where $v_c(q)=4\pi e^2/q^2$ is the Coulomb potential.

Various approaches to obtain expressions of the local field factor were investigated in the past [4–10]. Moroni *et al.* [4] obtained, by quantum Monte Carlo (QMC) simulation, the zero temperature local field factor $G(q)$ of the homogeneous electron gas at densities n_o corresponding to $r_s=2,5,10$ ($n_o=3/(4\pi a_B^3 r_s^3)$, where a_B is the Bohr radius). They also gave an analytical formula for $G(q)$ which fits the QMC computed value, and has the right asymptotic limits at small and large wave vector, *i.e.*:

$$G(q)\sim AQ^2 \qquad for\ \ q\rightarrow 0, \tag{3}$$

where $Q=q/k_F$, k_F is the Fermi wave vector,

$$A=\frac{1}{4}-\frac{k_F^2}{4\pi e^2}\frac{d\mu_c}{dn_o}, \tag{4}$$

μ_c being the correlation contribution to the chemical potential; and

$$G(q) \sim CQ^2 + B \qquad for \;\; q \to \infty, \tag{5}$$

where

$$C = \frac{\pi}{2e^2 k_F} \frac{-d(r_s \epsilon_c)}{dr_s}, \tag{6}$$

and ϵ_c is the correlation energy per particle. In our calculations we use the parametrization of B from Ref. [4]:

$$B(r_s) = \frac{(1 + a_1 x + a_2 x^3)}{(3 + b_1 x + b_2 x^3)}, \tag{7}$$

where $x = r_s^{1/2}$, $a_1 = 2.15$, $a_2 = 0.435$, $b_1 = 1.57$, and $b_2 = 0.409$, valid for r_s in the range 2–10 [11].

The Q^2 behaviour of the local-field factor at large Q has been overlooked for a long time. It has been demonstrated in Ref. [12], and a clear discussion of its origin is presented in Ref. [4]: its coefficient C is related to the change in kinetic energy in going from non-interacting (Kohn-Sham) electrons to interacting (real) electrons.

In this paper we fit the values of $G(q)$ computed in Ref. [4] in such a way to obtain a simple analytical expression of both $K_{xc}^{FT}(q)$ and $K_{xc}(r)$, where $K_{xc}(r)$ is the exchange correlation kernel in real space. Our formula for $G(q)$ is based on Lorentzian and Gaussian functions, and reads:

$$G(q) = CQ^2 + \frac{BQ^2}{g + Q^2} + \alpha Q^4 e^{-\beta Q^2}, \tag{8}$$

where $g = B/(A - C)$ and the two parameters α and β are fitted in order to minimize the differences with the numerical results of Ref. [4]. In particular, the best results are obtained taking:

$$\alpha = \frac{1.5}{r_s^{\frac{1}{4}}} \frac{A}{Bg}, \tag{9}$$

$$\beta = \frac{1.2}{Bg}. \tag{10}$$

Note that the Lorentzian contribution in Eq.8 is a simple Hubbard-like term. This term alone yields already *qualitative* agreement with the numerical data of Ref. [4]. Adding the Gaussian term allows us to reproduce *quantitatively* the numerical evaluation of Ref. [4]. In panels *a*, *b*, and *c* of Fig.1, $G(q)$ given by Eq.8 is compared with the QMC results of Ref. [4] for the unpolarized electron gas. The agreement is satisfactory, and is globally of the same quality as that obtained with the interpolation formula originally proposed in Ref. [4]. In panel *d* of Fig.1, we extend the comparison to QMC data for the fully spin polarized electron gas at $r_s = 100$ [13]. Despite the fact that this value is well beyond the range considered in Ref. [4] for the parametrization of B (Eq.7), and that in Eq.8 we neglect spin polarization effects, the agreement is still fairly good.

Using Eq.2, and after Fourier transforming, we obtain the expression of the exchange correlation kernel $K_{xc}(r)$ in real space:

$$K_{xc}(r) = -\frac{4\pi e^2 C}{k_F^2}\delta^3(r) + \frac{\alpha k_F}{4\pi^2\beta}(\frac{\pi}{\beta})^{\frac{3}{2}}[\frac{k_F^2 r^2}{2\beta} - 3]e^{-\frac{k_F^2 r^2}{4\beta}} - B\frac{e^{-\sqrt{g}k_F r}}{r}. \tag{11}$$

In Fig.2, we compare this form of K_{xc} (without the first term, which contains a three-dimensional delta function) with the (numerical) FT of the kernel derived from the Utsumi and Ichimaru parametrization of $G(q)$ [5]. Besides the very desirable property of allowing passage from real to reciprocal space and vice–versa without numerical transforms, the present form has another advantage, which is particularly useful in calculations for real solids: the absence of long-range oscillations, at variance with the case of those $G(q)$ which contain a logarithmic singularity for $q = 2k_F$, as the Ichimaru-Utsumi one (see Fig.2). This singularity is a peculiar property of the homogenous electron gas, originating from its spherical Fermi surface and from the absence of a gap between filled and empty states. Even in the HEG, its existence is not certain, and it is likely not present in real materials [14]. Hence it is better, given the present level of ignorance about the exchange-correlations kernel of real materials and the computational difficulties arising from such a singularity, to use expressions of $G(q)$ which do not contain it, and consequently do not yield the long range oscillations of $K_{xc}(r)$.

In conclusion, we have presented a new parametrization of published QMC results for the local field factor $G(q)$ of the homogeneous electron gas. Our analytical form fits the numerical data with the same accuracy as the form originally proposed in Ref. [4], has the right limiting behaviours for large and small q, and has the additional advantage of being analytically Fourier-transformable, a property which greatly simplifies its use in density-functional calculations for real materials.

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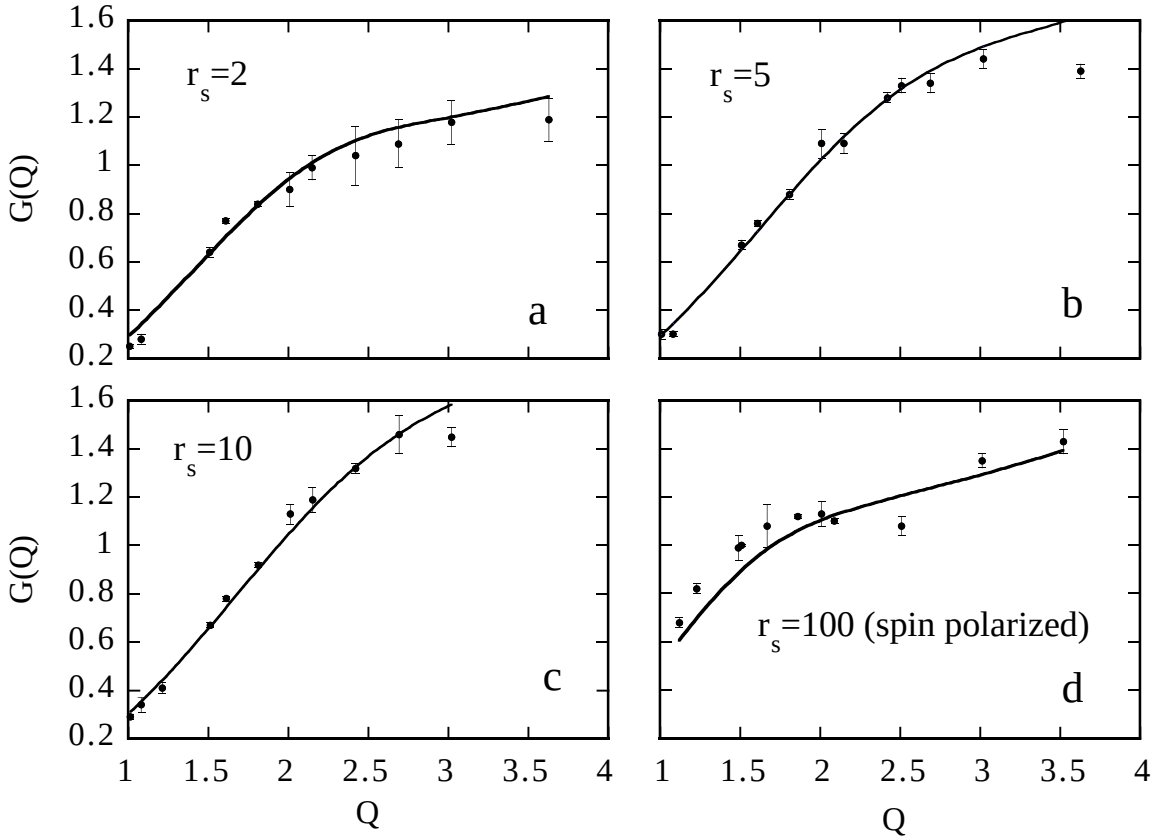
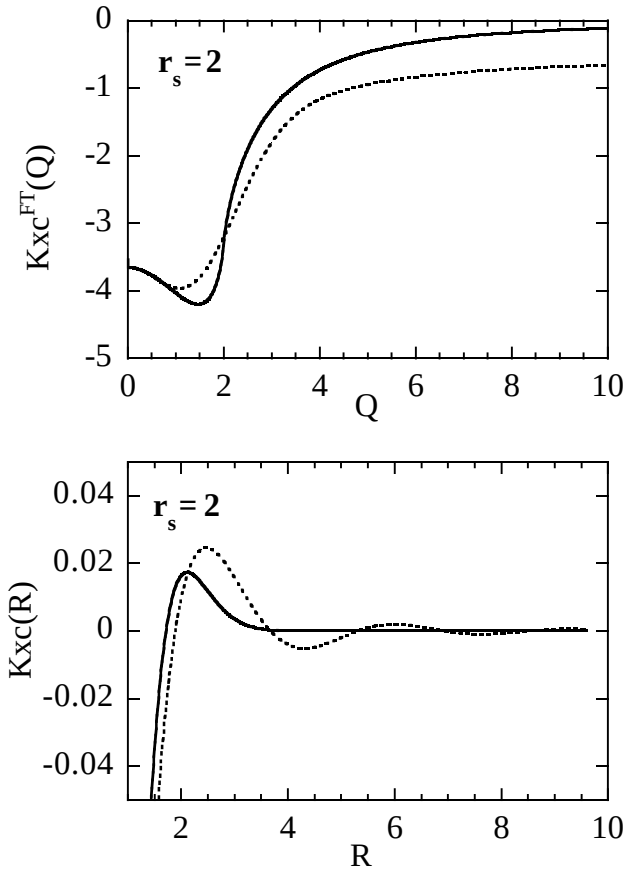
[14] A plateau or weak minimum at about $k = 2.5k_F$, which could be related to such a singularity, is present only in the QMC data for the spin polarized HEG at $r_s = 100$ (Fig. 1 *d*).

FIG. 1. Panels *a*, *b*, and *c*: local field factor $G(Q)$, ($Q = q/k_F$) as computed according to Eq. 8, in comparison with the QMC data for the unpolarized HEG of Ref. [4]. Panel *d*: Eq.8 compared with QMC data for the fully spin polarized HEG [13].

FIG. 2. The exchange-correlation kernel K_{xc} of the homogeneous electron gas as parametrized in the present work (full line), compared with the K_{xc} of Ref. [5] (dotted line), in atomic units, plotted in reciprocal and direct space (upper and lower panel, respectively, with $Q = q/k_F$ and $R = rk_F$)


G(Q)
Q
r_s=2
a
r_s=5
b
r_s=10
c
r_s=100 (spin polarized)
d
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
1
1.5
2
2.5
3
3.5
4


$r_s = 2$
$K_{XC}^{FT}(Q)$
Q
$r_s = 2$
$K_{XC}(R)$
R